

# Automating the Process of Invention

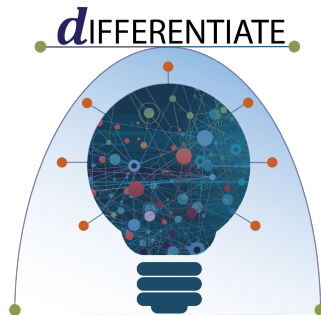
## Fast Pitch

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Advanced Research Projects Agency – Energy (ARPA-E)

# Automating the Process of Invention

*By leveraging the transformational potential of **machine learning (ML)***



## ARPA-E Mission

**Mission:** To overcome long-term and high-risk technological barriers in the development of energy technologies

Ensure U.S.  
Technological Lead &  
U.S. Economic and  
Energy Security

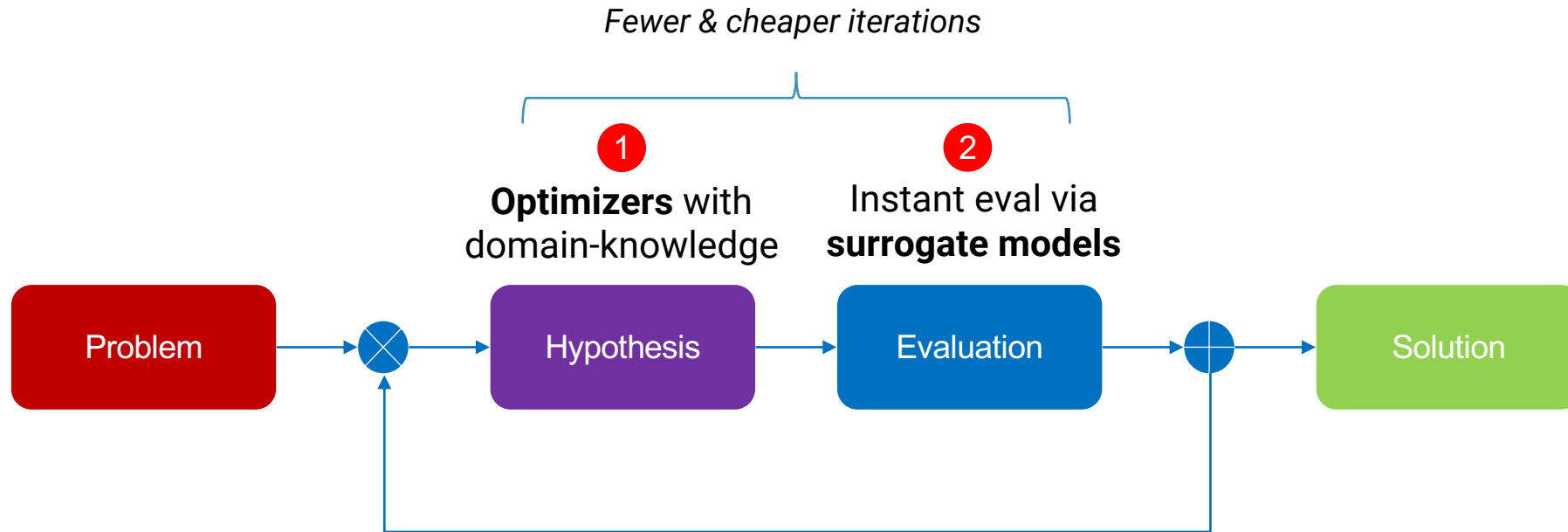


arpa-e

*Today's Focus: Progress, Challenges & Potential Next Steps*

# Design Process Framework & Targeted Capabilities

*Goal: Develop better technologies faster*



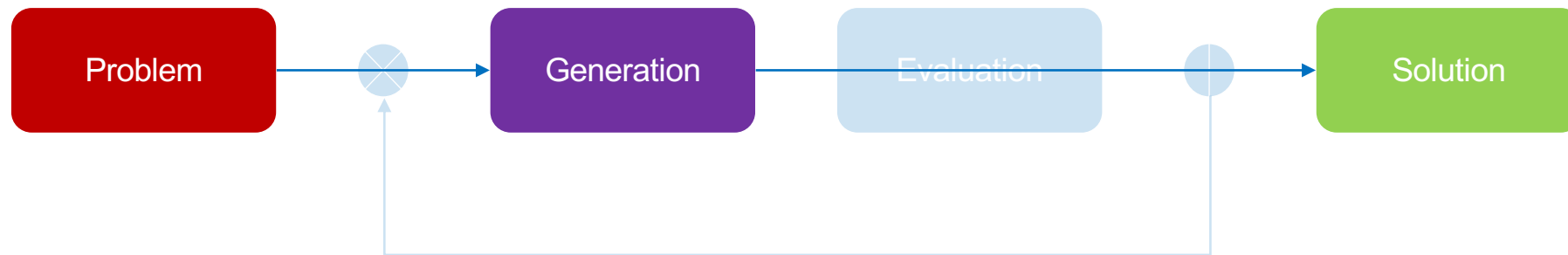
1 → Fewer iterations

2 → Faster evaluations

# Design Process Framework & Targeted Capabilities

*Goal: Develop better technologies faster*

3 Instant designs via **generative models**



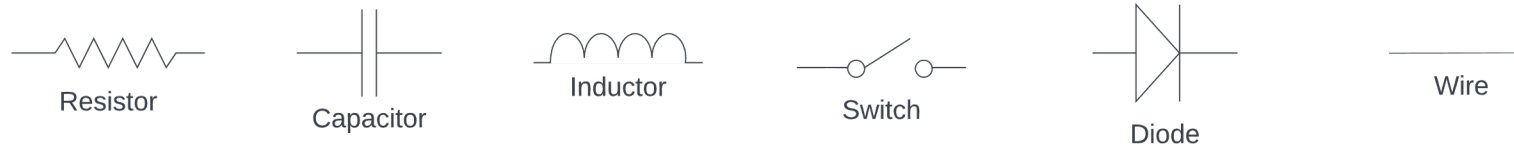
3 → Get it right the first time

# Progress: Domain Expert Optimizers

1



*D' Focus Area: Combinatorial optimization of thermodynamic systems, electrical circuits, materials*



*Design questions*

*D' Question*

*Which components? What specs? How connected? → Can we teach an algorithm to answer these questions?*

# Circuit Design via Reinforcement Learning (RL)

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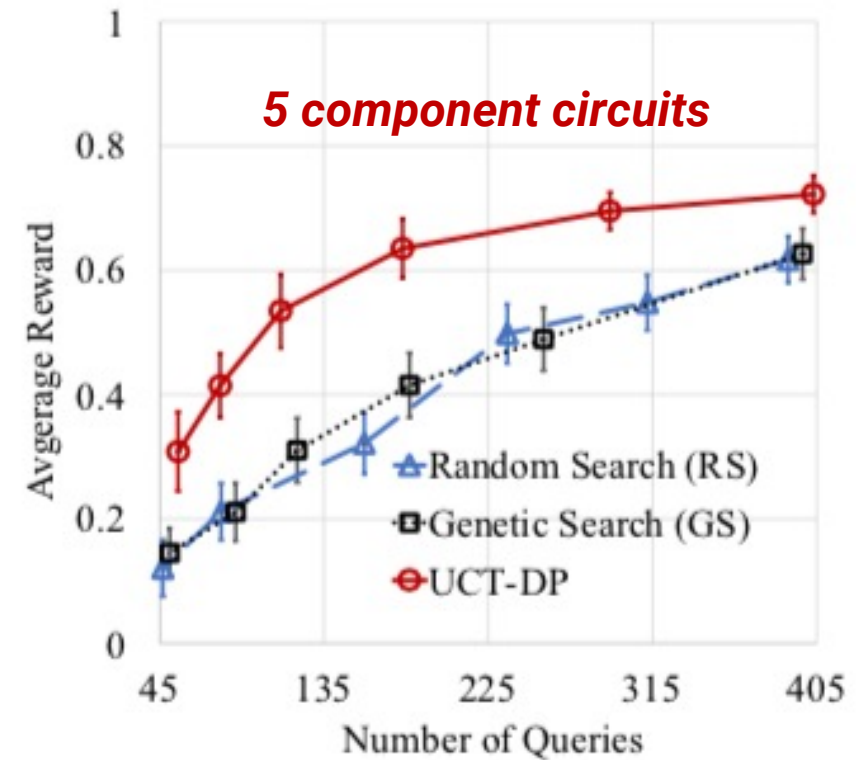


## Learning Process

- Build & evaluate many circuit concepts
  - Components
  - Connections (Wires)
  - Controls (Switch Timing)
- RL algorithms learn to maximize “reward”
  - Efficiency
  - Cost
  - NPV

Examples

## RL (UCT-DP) vs SOA



(a) Buck-Boost Converter

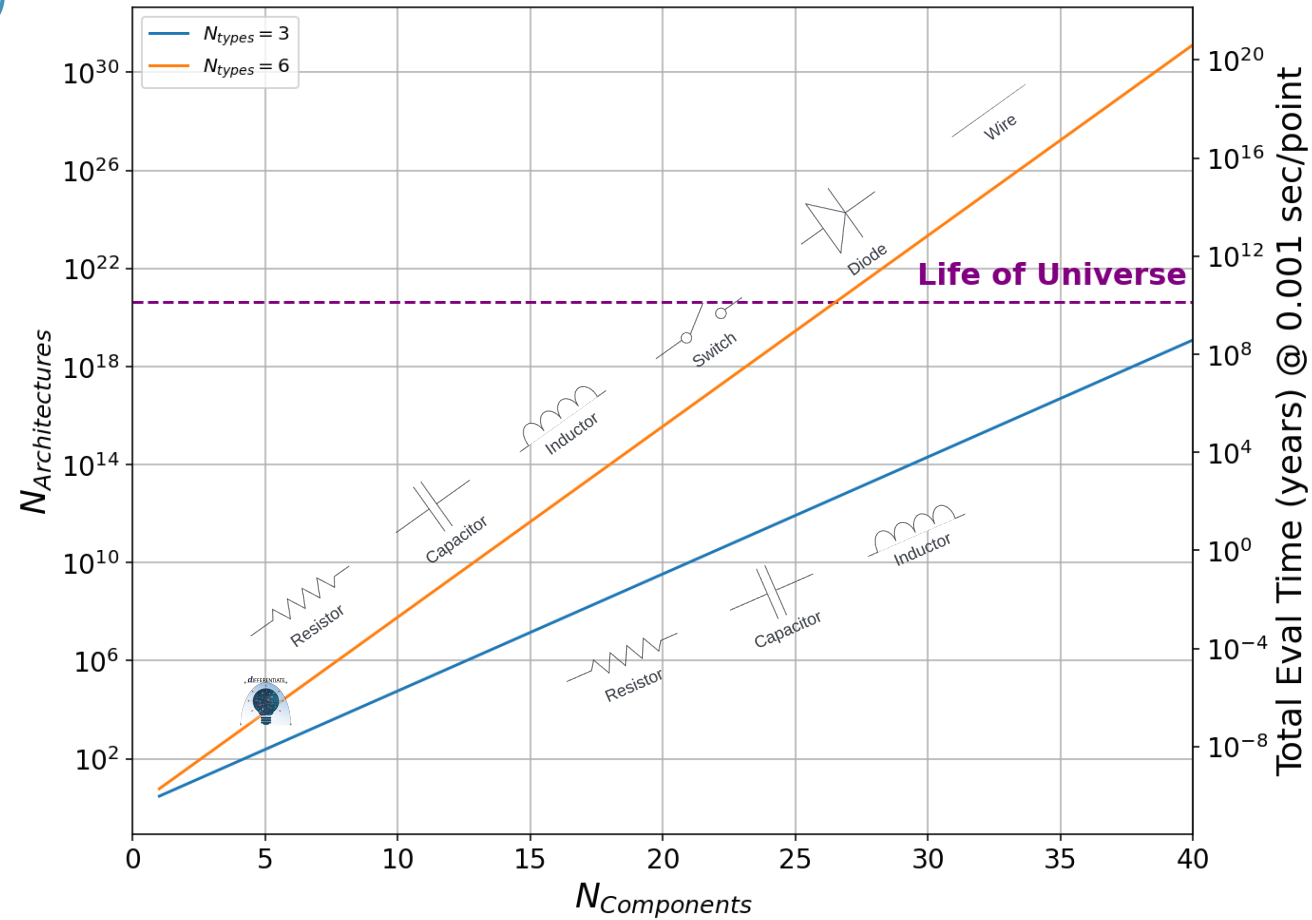
# Complexity Challenge: Combinatorial Explosion\*

\*Lighthill, James, "Artificial Intelligence: A General Survey", 1973

1

Enormous design space. Most choices are bad.

$$N_{\text{architectures}} = (N_{\text{types}})^{N_{\text{components}}}$$



High-Level Mitigations

1. Learn to make good choices
2. Efficiently weed out bad ones

# Emerging Complexity Management Solutions

1 2 3



*Goal: Reduce cost/amount of training data*

- ▶ **Leverage existing knowledge**

- Rules to enable rapid disposition of ‘bad’ ideas (e.g., no short circuits)
- Structured algorithms (e.g., GNNs) that respect physics & architectures

- ▶ **Leverage existing data**

- Historical data (good & bad)
- Previously trained (NN) algorithms (transfer learning)

- ▶ **Focus on what’s important**

- Dimensionality reduction



# Takeaways

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- ▶ ML methods offer potential for attractive design value propositions
  - **Domain expert optimizers**
  - Surrogate models
  - Generative/inverse models
- ▶ Challenge is management of 'real-world-scale' complexity
  - Leverage physics to simplify ML representations & reduce training cost
  - Learn when/how to transfer knowledge between applications/tools
  - ...
- ▶ Ideas? Please reach out: [david.tew@hq.doe.gov](mailto:david.tew@hq.doe.gov)

